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In the first 18 months of the Contract we have made fundamental progress in the identification of point defect complexes in semiconductors (particularly EL2 and EL0 in GaAs), the elucidation of the mechanisms by which they migrate (particularly re vacancy nearest neighbor hopping in compound semiconductors and recombination enhanced migration of vacancies in Si), and the development of an efficient means to simulate their detailed, and very complicated, diffusion and inter-reaction on a microcomputer using an inovative (and evidently unique) Monte Carlo method. Some effort (in collaboration with Dr. Kevin Malloy of AFOSR) has also recently gone into the elucidation of the temperature dependence of band off sets at heterojunctions, particularly GaAs-AlAs and HgTe-CdTe.

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18 MONTH TECHNICAL REPORT

to

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

BOLLING AIR FORCE BASE, D. C. 20332

POINT DEFECTS IN SEMICONDUCTORS: MICROSCOPIC IDENTIFICATION, METASTABLE PROPERTIES, DEFECT MIGRATION, AND DIFFUSION.

(AFOSR-86-0309)

For Period

31 August 1986 to 29 February 1988

Submitted by

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and

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In the first 18 months of the Contract we have made fundamental progress in the identification of point defect complexes in semiconductors (particularly EL2 and ELO in GaAs), the elucidation of the mechanisms by which they migrate (particularly re vacancy nearest neighbor hopping in compound semiconductors and recombination enhanced migration of vacancies in Si), and the development of an efficient means to simulate their detailed, and very complicated, diffusion and inter-reaction on a microcomputer using an innovative (and evidently unique) Monte Carlo method. Some effort (in collaboration with Dr. Kevin Malloy of AFOSR) has also recently gone into the elucidation of the temperature dependence of band off sets at heterojunctions, particularly GaAs-AlAs and HgTe-CdTe.

Our model of the metastable defect complex EL2 in GaAs, which originated prior to the Contract, has been refined, defended from criticism (see Reply to Comment of von Bardeleben, et al.), and extended to treat the distinct, but related, O containing complex known as ELO. Although there is still controversy over the subject, it is now turning to the details of the configuration of the As antisite (As/Ga/), Ga vacancy (V/Ga/), and As vacancy (V/As/) complex that we proposed and to questions of who thought of the correct model first. (See Comment of Zou et al.) We are more concerned with the question just how it forms during sample processing and whether its formation must be catalyzed, either by dislocations or by amphoteric impurities, such as C or Si. To date our Monte Carlo simulations seem to imply that the formation of EL2 from isolated point defects (two V/Ga/'s) must be catalyzed, but we are not yet confident of that conclusion. Resolution of that question will require further development of our treatment of electrostatic interactions between the migrating point defect complexes, as described below.

We devised a critical experiment to test our previously developed theory, the "Ballistic Model", for the activation enthalpy of vacancy nearest neighbor hopping. This experiment involved variable temperature, bias-stress measurements on InP MIS capacitors. InP is particularly useful to test this theory because its cation, In, is about 4 times heavier than its anion, P. Our theory immediately predicted from this fact that the activation enthalpy for V/P/ nearest neighbor hopping should be 4 times greater than for V/In/ nearest neighbor hopping, and further that their values should be about 1.2 eV and 0.3 eV. Other theories had predicted that the values should either be about equal or greater for the V/In/. There had been good evidence that the activation enthalpy for V/In/ was indeed about 0.3 eV but that for V/P/ migration was either regarded as unknown or ascribed to a 0.038 or 0.016 eV activation energy deduced from drain current drift measurements on InP MISFET's. Prior to our work on the Contract, no activation enthalpy of order 1.2 eV had been reported for any defect migration process in InP.

The experiment itself was innovative in that the physics of the capacitor interfaces had to be carefully analyzed. We developed computer simulations of such effects as the flat band shift as a function of stress time, which previously had generally not been considered by those practicing the technique. We demonstrated, to the satisfaction of a lively session of an Electrochemical Society Semiannual meeting and to the referees of the Journal of

the Electrochemical Society, that the flat band shift under bias stress above room temperature is clearly related to V/P/ nearest neighbor hopping and that the activation enthalpy for that process is 1.1 to 1.2 eV. The 38 meV and 16 meV processes observed in drain current drift at temperatures well below room temperature most probably involve tunneling of electrons into within the native oxide present at the SiO / InP interface.

We also made a fundamental extension of the "Ballistic Model" theory for atomic migration by deriving the first and only quantitative account of the activation enthalpy of recombination-enhanced vacancy migration, as a function of vacancy charge state, in Si at low temperatures. The recombination-enhanced migration of single vacancies in Si has been observed, particularly by George Watkins, for several years. Similar recombination-enhanced migration of vacancies and impurity interstitials have been observed by several groups in several semiconductors. The Ballistic Model gives definite values for the total enthalpy required for the migration process. When this is combined with empirical values of the defect ionization levels, to determine the amount of recombination energy delivered to the lattice, that can pay part or all the price required, the difference, if any, is our predicted activation enthalpy for the process in the presence of recombination. The agreement between this theory and the low temperature data of Watkins is quite satisfactory.

This theory of the recombination enhanced migration of point defects has also been extended to (high) semiconductor processing temperatures. There the effect had not previously been discussed. We show that the rate of recombination of thermal electrons and holes is orders of magnitude larger than the injection-induced recombination used in any of the low temperature experiments where recombination enhanced defect migration is commonly observed. Thus, the effect of thermal charge fluctuations at point defects may make a significant contribution to their net diffusivity during processing. We show that the well established but highly controversial temperature dependence of the activation enthalpy for self diffusion in Si, between 4.0 and 5.2 eV, may be explained in this way.

Our Monte Carlo simulation program of point defect migration and interaction continues to develop. We had not appreciated the importance of the charge state fluctuations just described to the problem of the high temperature simulation when we began the project. We are still working on the proper incorporation of that effect into the program. In the meantime, we have the program running (sans electrostatic interaction) with vacancies allowed to hop to either first or second neighbor sites. An extension of the program to simulate host or impurity interstitials allowed to hop among bond centered, tetrahedral or hexagonal interstitial sites and to vacant lattice sites has been written and is now being debugged. We will soon be able to allow the spontaneous creation of vacancy-interstitial pairs and to simulate the "kick-out" mechanism.

We have been using the Monte Carlo program for problems we believe to be relatively insensitive to electrostatic interactions and to participation of interstitials. There have been three of these. One has been the problem of the interaction of

two V/Ga/'s to form an EL2 complex, as mentioned above. Another has been the effect of high energy (16 MeV) electron irradiation, which creates divacancies in GaAs, on the single vacancy concentration observed by positron annihilation in GaAs. Empirically the effect is to reduce the concentration of single vacancies, which was counter-intuitive to those who did the experiment. We showed that the effect of introducing excess divacancies was to promote the gettering of single vacancies into multiple vacancy complexes. This occurs even at room temperature, where the grown-in vacancies are greatly in excess of thermal equilibrium but rather immobile. It is likely that the gettering process is greatly enhanced by recombination enhancement during the radiation, has mentioned above. The third has been a study of the melting of Si and GaAs, which is simulated by placing a cluster (typically 48) of vacancies in the center of the sample to represent the free surface required for the nucleation of melting. This may be regarded as a test of the interatomic constants we have been assuming to represent the GaAs and the Si.

The results of our activity are discussed in detail in the attached reprints and preprints.